

On the bound states in the muonic molecular ions

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(Dated: August 29, 2012)

Abstract

The mass corrections to the bound state energies of the three-body muonic molecular ions $pp\mu$, $pd\mu$, $pt\mu$, $dd\mu$, $dt\mu$ and $tt\mu$ are determined numerically from the results of highly accurate computations. The total energies and some other bound state properties of these ions are evaluated to very high accuracy for the bound $S(L=0)$ -, $P(L=1)$ - and $D(L=2)$ -states. In these highly accurate calculations we used the most recent and accurate masses of particles m_p, m_d, m_t and m_μ known from high energy experiments. We also investigate some bound state properties of the muonic molecular ions. In particular, we determine the hyperfine structure splittings of the ground states of the $pd\mu$, $pt\mu$ and $dt\mu$ ions. In these calculations we used our highly accurate expectation values of the interparticle delta-functions obtained in recent computations. The corresponding hyperfine structure splittings, e.g., $\Delta_{12} = 1.3400149 \cdot 10^7$ MHz and $\Delta_{23} = 3.3518984 \cdot 10^7$ MHz for the $pt\mu$ ion, can directly be measured in modern experiments. Analogous hyperfine structure splittings are evaluated to very high accuracy for all five bound $S(L=0)$ -states in the three symmetric muonic molecular ions: $pp\mu$, $dd\mu$ and $tt\mu$.

PACS number(s): 36.10.+Di, 36.10.-k and 31.10.+z.

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I. INTRODUCTION

In our earlier study [1] we considered the bound state spectra in the muonic molecular ions $pp\mu$, $pd\mu$, $pt\mu$, $dd\mu$, $dt\mu$ and $tt\mu$, where the notations p , d , t stand for the nuclei of three hydrogen isotopes (protium, deuterium and tritium, respectively), while μ means the negatively charged muon μ^- . In our calculations in [1] we have used the particle masses taken from relatively old experimental papers, since in [1] we wanted to show the progress achieved recently in highly accurate computations of Coulomb three-body systems with arbitrary masses. Therefore, it was some logic to use the same particle masses in all such calculations (see, e.g., [2], [3] and references therein). On the other hand, right now the masses of all nuclei of hydrogen isotopes (p , d and t) and negatively charged muon μ^- are known to much better accuracy, than they were obtained ten years ago (in fact, eighteen years ago). It is clear that it is necessary to perform extensive recalculations of the bound state energies and other bound state properties in the six muonic molecular ions $pp\mu$, $pd\mu$, $pt\mu$, $dd\mu$, $dt\mu$ and $tt\mu$ by using the ‘recently updated’ particle masses.

Modern highly accurate computations of the bound states in muonic molecular ions allow one to determine 15 - 18 correct decimal digits in the total energy E . In some cases, e.g, for the $S(L = 0)$ -state in the $pp\mu$ ion such an accuracy is much higher and we can determine ≈ 21 - 22 correct decimal digits in the total energy. On the other hand, the masses of particles have been determined to the accuracy which corresponds to ≈ 10 - 11 exact decimal digits only. Such uncertainties in particle masses lead to relatively large mistakes in the total energies and corresponding wave functions. Formally, this means an almost constant need of recalculation of the corresponding total energies and wave functions by solving the non-relativistic three-body Schrödinger equation with the new masses. Note also that in contrast with the two-electron atoms for three-body muonic molecular ions we cannot use various mass-interpolation formulas for the total energies, since they are not very accurate and contain not one, but two and even three different parameters (i.e. the ratios of the masses of particles) and none of these parameters is small.

The main goal of this study is to perform the highly accurate computations of the bound states in the six muonic molecular ions $pp\mu$, $pd\mu$, $pt\mu$, $dd\mu$, $dt\mu$ and $tt\mu$. All particle masses used in our calculations are taken from the most recent high energy experiments. Our calculations are performed with the use of extended arithmetic precision. Finally, the mass

corrections to the total energies of these ions have been determined (for each bound state in these six ions) to very high accuracy.

By using the highly accurate expectation values of all (three) interparticle delta-functions obtained in our calculations we also investigate the hyperfine structure of the bound $S(L = 0)$ —states in the six muonic molecular ions $pp\mu, pd\mu, pt\mu, dd\mu, dt\mu$ and $tt\mu$. The hyperfine structure splittings are determined for each of these (nine) bound $S(L = 0)$ —states. The results of this investigation lead us to a number of interesting conclusions and observations. Many of these facts are important in analogous computations of more complicated systems, e.g., in the analysis of hyperfine structure splittings in the four-, five- and six-body quasi-atoms and ions which contain muonic molecular ions as a part of their structure.

II. THE MASS-DEPENDENT HAMILTONIAN OF MUONIC MOLECULAR IONS

In the non-relativistic approximation the Hamiltonian of the three-body muonic molecular ion $ab\mu$ (or $(ab\mu)^+$) takes the form

$$H = -\frac{\hbar^2}{2m_\mu} \left(\frac{m_\mu}{m_a} \nabla_a^2 + \frac{m_\mu}{m_b} \nabla_b^2 + \nabla_\mu^2 \right) + \frac{q_a q_b e^2}{r_{ab}} + \frac{q_a q_\mu e^2}{r_{a\mu}} + \frac{q_b q_\mu e^2}{r_{b\mu}} \quad (1)$$

where $\nabla_i = \left(\frac{\partial}{\partial x_i}, \frac{\partial}{\partial y_i}, \frac{\partial}{\partial z_i} \right)$ and $i = a, b, \mu$. In Eq.(1) \hbar is the reduced Planck constant ($\hbar = \frac{h}{2\pi}$) and e is the elementary electric charge. It is very convenient (see below) to consider the bound state spectra of such ions in muon-atomic units in which $\hbar = 1, m_\mu = 1$ and $e = 1$. The speed of light c in these units is $c = \alpha^{-1}$, where $\alpha = \frac{e^2}{\hbar c}$ is the fine structure constant. In muon-atomic units the same Hamiltonian, Eq.(1), is written in the form

$$H = -\frac{1}{2} \left(\frac{1}{m_a} \nabla_a^2 + \frac{1}{m_b} \nabla_b^2 + \nabla_\mu^2 \right) + \frac{1}{r_{ab}} - \frac{1}{r_{a\mu}} - \frac{1}{r_{b\mu}} \quad (2)$$

where the nuclear masses m_a and m_b of the two hydrogenic nuclei must be expressed in terms of the muon mass m_μ .

In our earlier studies (see, e.g., [1], [2] and references therein) we used the following masses of the hydrogenic nuclei p, d, t and negatively charged muon μ

$$\begin{aligned} m_\mu &= 206.768262 m_e \quad , \quad m_p = 1836.152701 m_e \\ m_d &= 3670.483014 m_e \quad , \quad m_t = 5496.92158 m_e \end{aligned} \quad (3)$$

where m_e designates the electron mass. In particular, these masses were used in our earlier studies (see, e.g., [2], [3] and references therein). In this work the updated values for the nuclear masses of all four particles p^+, d^+, t^+ and μ^- will be used. The masses of these four particles have recently been determined in various high-energy experiments to better accuracy than they were known in the middle of 1990's. Usually, these masses are expressed in special high-energy mass units MeV/c^2 . In these high-energy units the corresponding masses are

$$\begin{aligned} m_\mu &= 105.65836668(38) \quad , \quad m_p = 938.272046(21) \\ m_d &= 1875.612859(41) \quad , \quad m_t = 2808.290906(70) \end{aligned} \quad (4)$$

These values include current experimental uncertainties. They are very close to the masses of these particles given in [16]. In all calculations performed in this study we have used the following masses of the μ, p, d and t particles (in MeV/c^2)

$$\begin{aligned} m_\mu &= 105.65836668 \quad , \quad m_p = 938.272046 \\ m_d &= 1875.612859 \quad , \quad m_t = 2808.290906 \end{aligned} \quad (5)$$

These values are considered as exact. The corresponding corrections to these masses can be taken into account by performing direct variational computations with the ‘new’ masses.

Since our calculations of muonic molecular ions are performed in muon-atomic units, then we need to use only three following mass ratios $\frac{m_\mu}{m_p}, \frac{m_\mu}{m_d}$ and $\frac{m_\mu}{m_t}$. These mass ratios are, in fact, the dimensionless parameters which determine the energy spectra and all other properties of the six muonic molecular ions $pp\mu, pd\mu, pt\mu, dd\mu, dt\mu$ and $tt\mu$. The total energies and the corresponding wave functions of the muonic molecular ions are determined during the highly accurate solution of the non-relativistic Schrödinger equation $H\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = E \cdot \Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$, where $E < 0$ and the non-relativistic Hamiltonian of the three-body system which is written in the form of Eq.(2). To determine the highly accurate solutions of the non-relativistic Schrödinger equation with $E < 0$ in this study we apply the exponential variational expansion in the relative/perimetric three-body coordinates. The explicit form of the exponential variational expansion in perimetric coordinates is

$$\Psi_{LM} = \frac{1}{2}(1 + \kappa \hat{P}_{21}) \sum_{i=1}^N \sum_{\ell_1} C_i \mathcal{Y}_{LM}^{\ell_1, \ell_2}(\mathbf{r}_{31}, \mathbf{r}_{32}) \exp(-\alpha_i u_1 - \beta_i u_2 - \gamma_i u_3) \quad (6)$$

where C_i are the linear (or variational) parameters, $\alpha_i, \beta_i, \gamma_i$ are the non-linear parameters and L is the angular momentum of the three-body system $ab\mu$. Note that each basis function in Eq.(6) is an eigenfunction of the L^2 and L_z operators with eigenvalues $L(L+1)$ and M . This means that $\hat{L}^2\Psi_{LM} = L(L+1)\Psi_{LM}$, while M is the eigenvalue of the \hat{L}_z operator, i.e. $\hat{L}_z\Psi_{LM} = M\Psi_{LM}$. The operator \hat{P}_{21} in Eq.(6) is the permutation of the two identical particles in symmetric three-body systems. For such systems in Eq.(6) one finds $\kappa = \pm 1$, otherwise $\kappa = 0$. In general, for the bound states of natural spatial parity we chose in Eq.(6) $\kappa = (-1)^L$ for all symmetric muonic molecular ions $pp\mu, dd\mu, tt\mu$ and $\kappa = 0$ for all non-symmetric ions $pd\mu, pt\mu, dt\mu$.

The functions $\mathcal{Y}_{LM}^{\ell_1, \ell_2}(\mathbf{r}_{31}, \mathbf{r}_{32})$ in Eq.(14) are the bipolar harmonics [5] of the two vectors $\mathbf{r}_{31} = r_{31} \cdot \mathbf{n}_{31}$ and $\mathbf{r}_{32} = r_{32} \cdot \mathbf{n}_{32}$. The bipolar harmonics are defined as follows [5]

$$\mathcal{Y}_{LM}^{\ell_1, \ell_2}(\mathbf{x}, \mathbf{y}) = x^{\ell_1} y^{\ell_2} \sum_{\ell_1, \ell_2} C_{\ell_1 m_1; \ell_2 m_2}^{LM} Y_{\ell_1 m_1}(\mathbf{n}_x) Y_{\ell_2 m_2}(\mathbf{n}_y) \quad (7)$$

where $C_{\ell_1 m_1; \ell_2 m_2}^{LM}$ are the Clebsch-Gordan coefficients (see, e.g., [5] and [6]) and the vectors $\mathbf{n}_x = \frac{\mathbf{x}}{x}$ and $\mathbf{n}_y = \frac{\mathbf{y}}{y}$ are the corresponding unit vectors constructed for arbitrary non-zero vectors \mathbf{x} and \mathbf{y} . As follows from Eq.(7) each bipolar harmonic is the M -component of the irreducible tensor of rank L . In actual calculations it is possible to use only those bipolar harmonics for which $\ell_1 + \ell_2 = L$. Note that the basis set, Eq.(6), is a partial case of the more general exponential variational expansion in the relative/perimetric coordinates [1]. In particular, our Eq.(14) does not include exponents with the imaginary (or complex) non-linear parameters and some other factors which are needed to accelerate the overall convergence rate for some three-body systems, e.g., for the H_2^+ , D_2^+ ions, helium-muonic atoms and for other ‘special’ systems (for more details, see, [1] and [7]). We also do not want to discuss here the bound states of unnatural spatial parity, when one needs to use in Eq.(6) the bipolar harmonics for which $\ell_1 + \ell_2 = L + 1$.

III. SPECTRA OF BOUND STATES IN MUONIC MOLECULAR IONS

By analyzing the bound state spectra in the six muonic molecular ions $pp\mu, pd\mu, pt\mu, dd\mu, dt\mu$ and $tt\mu$ one finds that they can be separated into three different groups [2] on qualitative grounds. The first group includes three light muonic molecular ions $pp\mu, pd\mu$ and $pt\mu$. Each of these systems has two bound states: one $S(L=0)$ -state

and one $P(L = 1)$ –state. Neither of these two states is weakly bound. Note that each of these light muonic molecular ions contains at least one protium nucleus. The second group includes the two ‘intermediate’ muonic molecular ions $dd\mu$ and $dt\mu$ each of which has five bound states: two $S(L = 0)$ –states, two $P(L = 1)$ –states and one $D(L = 2)$ –state. One of these five states (the excited $P^*(L = 1)$ –state in each of these two ions) is weakly bound. By the formal definition the weakly bound state in a few-body system is a state with very small binding energy ε , or, in other words, with a very small ratio of the binding and total energies, i.e., $\tau = \frac{\varepsilon}{E} \ll 1$, where τ is the dimensionless parameter. The third group contains only the heaviest muonic molecular ion $tt\mu$ which has six bound states (and no weakly bound states): two $S(L = 0)$ –states, two $P(L = 1)$ –states, one $D(L = 2)$ –state and one $F(L = 3)$ –state.

The classification of bound state spectra in muonic molecular ions is based on the general theory developed in [8], [9] for three-body Coulomb systems with unit charges. This theory is based on the fact that the total number of bound states in any muonic molecular ion $a^+b^+\mu^-$ is determined by the lightest nucleus of the hydrogen isotope in this ion. This explains why only three groups of different bound state spectra can be found in the six muonic molecular ions mentioned above: the p –group, the d –group and the t –group. Furthermore, it must be a similarity between the spectra of bound states in each group: e.g., between the bound state spectra of the ‘protium’ muonic molecular ions $pp\mu$, $pd\mu$ and $pt\mu$. Analogous similarity can be found for the bound state spectra of the $dd\mu$ and $dt\mu$ ions in the ‘deuterium’ group. It can be shown that in such ‘families’ of muonic molecular ions the symmetric ion always has the maximal binding energy [9]. By using these similarities between the bound state spectra in each of these ‘families’, one also finds a number of useful relations for the total and binding energies as well as for other bound state properties of different muonic molecular ions (see examples in [1]).

As we have mentioned above there are 22 bound states in the six muonic molecular ions $pp\mu$, $pd\mu$, $pt\mu$, $dd\mu$, $dt\mu$ and $tt\mu$. Nine of these states are the $S(L = 0)$ –states, while nine others are the $P(L = 1)$ –states. There are also three bound $D(L = 2)$ –states and one bound $F(L = 3)$ –state. The F –state is stable only in the heavy $tt\mu$ ion. In this study we determine the total energies of twenty one such bound states. At this moment we cannot perform the highly accurate computations of the $F(L = 3)$ –state in the $tt\mu$ ion, since our unique code for such calculations was lost a few months ago (due to some problems at our

local computer).

IV. RESULTS AND DISCUSSIONS

In this study all numerical computations of the S - and P -bound states in muonic molecular ions in this study are performed with the use of 64 - 108 decimal digits per computer word [10], [11], allowing the total energies to be determined to the accuracy $\approx 1 \cdot 10^{-21} - 1 \cdot 10^{-23} \text{ m.a.u.}$ In all calculations we have assumed that all particle masses and corresponding conversion factors (e.g., the factor Ry mentioned below) are exact. In fact, such assumptions are always made in the papers on highly accurate computations in few-body systems (see, e.g., [12] and [13]). The known experimental uncertainties in particle masses and conversion factors are taken into account at the last step of calculations, when the most accurate computations are simply repeated for a few times with the use of different particle masses and conversion factors. Analogously, the expectation values of other operators are determined in calculations with our non-relativistic wave functions. To avoid a substantial loss of numerical accuracy during computations of the expectation values of some operators these non-relativistic wave functions must be extremely accurate.

Table I contains the total variational energies obtained for the ground and first ‘vibrationally’ excited $S(L = 0)$ -states of the symmetric and non-symmetric muonic molecular ions $pp\mu, pd\mu, pt\mu, dd\mu, dt\mu$ and $tt\mu$. Table II includes the total energies for the rotationally and vibrationally excited $P(L = 1)$ - and $P^*(L = 1)$ -states of these six muonic molecular ions. In these two Tables and everywhere below the upper index ‘*’ is used to designate the vibrationally excited state with the same angular momentum L . Table III contains the total energies of the $D(L = 2)$ -states in the three heavy muonic molecular ion $dd\mu, tt\mu$ and $dt\mu$. The results from Table III have been obtained with the use of the standard Fortran with the quadruple precision accuracy (30 decimal digits per computer word). Also, in calculations of the bound $D(L = 2)$ -states we did not applied our two-stage optimization of the non-linear parameters in the trial wave functions. Therefore, the energies from Table III are less accurate than analogous energies from Tables I and II.

In Tables I - III the notation ∞ stands for the total energy which corresponds to the infinite number of basis function, i.e. $N = \infty$ in Eq.(14). The asymptotic formula for the

total energy takes the following four-parameteric form

$$E(N_i) = E(\infty) + \frac{A_1}{N_i^\gamma} + \frac{A_2}{N_i^{\gamma+1}} \quad (8)$$

where $E(\infty)$, A_1 , A_2 and γ are the four parameters which are determined by using the results of highly accurate calculations of the total energies with the different numbers of basis functions N_i (see Eq.(6)). To determine four parameters in Eq.(8) one needs to know at least four total energies $E(N_i)$ obtained from the direct numerical calculations. In general, the asymptotic value of the total energy contains one/two correct decimal digit(s) extra. Moreover, the exact coincidence of some decimal digits in the $E(N_i)$ and $E(\infty)$ energies in Eq.(8) allow us to confirm the total number of stable decimal digits in the final energies.

Highly accurate calculations of the total energies and other bound state properties for all known bound states in muonic molecular ions is an important and actual scientific problem. As mentioned above in this study we use the improved values of particle masses known from recent high energy experiments. Our results presented in Tables I - III provide answers for a number of actual questions. For instance, as is well known the bound $P^*(L = 1)$ -states in the $dd\mu$ and $dt\mu$ ions are very weakly bound. By using the corresponding energies from Table II and improved masses of the muon, deuterium and tritium nuclei (see above) one finds the ‘improved’ binding energies of the $P^*(L = 1)$ -states in the $dd\mu$ and $dt\mu$ ions:

$$\varepsilon(dd\mu; P^*(L = 1)) = -1.9749828376301(2)eV \quad (9)$$

and

$$\varepsilon(dt\mu; P^*(L = 1)) = -0.6603325645(2)eV \quad (10)$$

where we have used the following conversion factor $Ry = 27.211385060 \cdot \left(\frac{m_\mu}{m_e}\right)$ from muon-atomic units to electron volts ($1 eV = 1.602176487(40) \times 10^{-19} J$). Note that such a recalculation from muon-atomic units to electron volts requires the knowledge of the electron mass m_e ($m_e = 0.510\,998\,910\, MeV/c^2$) and Rydberg constant Ry (or conversion factor), The binding energies of any other bound state in muonic molecular ions can be evaluated analogously. These values can be compared with the binding energies $\varepsilon(dd\mu; P^*(L = 1))$ and $\varepsilon(dt\mu; P^*(L = 1))$ determined in [1].

Another interesting problem is to study the changes in the bound state properties of these muonic molecular ions which are directly related to the mass variations. The results of these calculations (in muon-atomic units) can be found in Table IV for some of the properties.

The results from this Table can be compared with analogous results from Table 8 given in [1]. Such a comparison shows the effect of mass variation for the bound states properties which are different from the total and binding energies. By working with Table IV we have found the numerical mistake in the $\langle r_{21}^2 \rangle$ expectation value for the $pd\mu$ ion (extra ‘1’ was added from the left side to this result in Table 8 in [1]). The mass corrections to the total energies can be obtained by subtracting our results from Table I - III from the corresponding results given in Tables 1 - 5 in [1]. Since the total energies in all these Tables are given in muon-atomic units, then we do not need to use any additional conversion factor.

V. HYPERFINE STRUCTURE OF THE GROUND STATES IN THE $pd\mu$, $pt\mu$ AND $dt\mu$ IONS

In this Section we analyze the hyperfine structure and determine the hyperfine structure splitting of the bound $S(L = 0)$ -states in the non-symmetric muonic molecular ions $pd\mu$, $pt\mu$ and $dt\mu$. As is mentioned above there are four bound $S(L = 0)$ -states in these three ions: three ground $S(L = 0)$ -states (one in each of these ions) and one excited $S(L = 0)$ -state in the heavy $dt\mu$ ion. In this Section we want to investigate the hyperfine structure and determine the hyperfine structure splitting for each of these bound states by using highly accurate expectation values of the delta-functions obtained in our highly accurate numerical computations (see above).

The general formula for the hyperfine structure splitting $(\Delta H)_{h.s.}$ (or hyperfine splitting, for short) in the case of an arbitrary three-body system is written as the sum of the three following terms. Each of these terms is proportional to the product of the factor $\frac{2\pi}{3}\alpha^2$ and expectation value of the corresponding (interparticle) delta-function. The third (additional) factor contains the corresponding g -factors (or hyromagnetic ratios) and scalar product of the two spin vectors. For instance, for the $pd\mu$ ion this formula takes the form (in atomic units) (see, e.g., [14], [15])

$$\begin{aligned}
 (\Delta H)_{h.s.} = & \frac{2\pi}{3}\alpha^2 \frac{g_p g_d}{m_p^2} \langle \delta(\mathbf{r}_{pd}) \rangle (\mathbf{s}_p \cdot \mathbf{s}_d) + \frac{2\pi}{3}\alpha^2 \frac{g_p g_\mu}{m_p m_\mu} \langle \delta(\mathbf{r}_{p\mu}) \rangle (\mathbf{s}_p \cdot \mathbf{s}_\mu) \\
 & + \frac{2\pi}{3}\alpha^2 \frac{g_d g_\mu}{m_p m_\mu} \langle \delta(\mathbf{r}_{d\mu}) \rangle (\mathbf{s}_d \cdot \mathbf{s}_\mu)
 \end{aligned} \tag{11}$$

where $\alpha = \frac{e^2}{\hbar c}$ is the fine structure constant, m_μ and m_p are the muon and proton masses, respectively. The factors g_μ , g_p and g_d are the corresponding g -factors. The expression

for $(\Delta H)_{h.s.}$ is, in fact, an operator in the total spin space which has the dimension $(2s_p + 1)(2s_d + 1)(2s_\mu + 1) = 12$. In our calculations we have used the following numerical values for the constants and factors from Eq.(11): $\alpha = 7.297352586 \cdot 10^{-3}$, $m_p = 1836.152701m_e$, $m_\mu = 206.768262m_e$ and $g_\mu = -2.0023218396$. The g -factors for the proton and deuteron are determined from the formulas: $g_p = \frac{\mathcal{M}_p}{I_p}$ and $g_d = \frac{\mathcal{M}_d}{I_d}$, where $\mathcal{M}_p = 2.792847386$ and $\mathcal{M}_d = 0.857438230$ are the magnetic moments (in nuclear magnetons) of the proton and deuteron, respectively. The spin of the proton and deuteron is designated in Eq.(11) as $I_p = \frac{1}{2}$ and $I_d = 1$.

The analogous formula for the hyperfine structure splitting in the $pt\mu$ ion takes the form

$$\begin{aligned} (\Delta H)_{h.s.} = & \frac{2\pi}{3}\alpha^2 \frac{g_p g_t}{m_p^2} \langle \delta(\mathbf{r}_{pt}) \rangle (\mathbf{s}_p \cdot \mathbf{s}_t) + \frac{2\pi}{3}\alpha^2 \frac{g_p g_\mu}{m_p m_\mu} \langle \delta(\mathbf{r}_{p\mu}) \rangle (\mathbf{s}_p \cdot \mathbf{s}_\mu) \\ & + \frac{2\pi}{3}\alpha^2 \frac{g_t g_\mu}{m_p m_\mu} \langle \delta(\mathbf{r}_{t\mu}) \rangle (\mathbf{s}_t \cdot \mathbf{s}_\mu) \end{aligned} \quad (12)$$

where $g_t = \frac{\mathcal{M}_t}{I_t}$, where $\mathcal{M}_t = 2.9789624775$ is the magnetic moment of the triton expressed in the nuclear magnetons and $I_t = \frac{1}{2}$ is the spin of the triton (or tritium nucleus). The formula for the hyperfine structure splitting in the $dt\mu$ ion is

$$\begin{aligned} (\Delta H)_{h.s.} = & \frac{2\pi}{3}\alpha^2 \frac{g_d g_t}{m_p^2} \langle \delta(\mathbf{r}_{dt}) \rangle (\mathbf{s}_d \cdot \mathbf{s}_t) + \frac{2\pi}{3}\alpha^2 \frac{g_d g_\mu}{m_p m_\mu} \langle \delta(\mathbf{r}_{d\mu}) \rangle (\mathbf{s}_d \cdot \mathbf{s}_\mu) \\ & + \frac{2\pi}{3}\alpha^2 \frac{g_t g_\mu}{m_p m_\mu} \langle \delta(\mathbf{r}_{t\mu}) \rangle (\mathbf{s}_t \cdot \mathbf{s}_\mu) \end{aligned} \quad (13)$$

where all values are defined above. The same formula can be applied to determine the hyperfine structure splitting in the excited $S(L = 0)$ -state of the $dt\mu$ ion. The only difference in the hyperfine structure splittings determined for the ground and excited states of the $dt\mu$ ion can be related with the expectation values of interparticle delta-functions.

In our computations of the muonic molecular ions performed recently [1] we have determined the expectation values of all delta-functions which are needed in Eqs.(11) - (13). The corresponding expectation values are shown in Table I. These values have been determined in muon atomic units where $m_\mu = 1, \hbar = 1, e = 1$. They must be re-calculated to the regular atomic units ($m_e = 1, \hbar = 1, e = 1$) which are used in the formulas, Eqs.(11) - (13), to determine the hyperfine structure splittings. In these calculations we have used the trial wave functions with $N = 3300, 3500, 3700$ and 3840 exponential basis functions (for more details, see [1]). The expectation values of all interparticle delta-functions computed for the ground $S(L = 0)$ -state of the $pd\mu$ ion are shown in Table I. The overall convergence rates of

the delta-functions computed for each bound state in the $pt\mu$ and $dt\mu$ ions are very similar to the results shown in Table V.

These expectation values of the $\delta(\mathbf{r}_{ij})$ functions were used in the formulas Eqs.(11) - (13) to determine the hyperfine structure splittings of the bound $S(L = 0)$ -states of the $pd\mu$, $pt\mu$ and $dt\mu$ ions. Numerical values of the corresponding hyperfine structure splittings can be found in Tables VI and VII. Note that these values are usually given in MHz , while the values of $(\Delta H)_{h.s.}$ which follow from Eqs.(11) - (13) are expressed in atomic units. To re-calculate them from atomic units to MHz the conversion factor $6.57968392061 \cdot 10^9 \text{ MHz}/a.u.$ was used [16].

In general, the $pd\mu$ and $dt\mu$ ions have similar hyperfine structure. In particular, in each of these ions one finds twelve spin states which are separated in the four following groups: (1) the group with $J = 2$ (five states), (2) the group with $J = 1$ (three states), (3) the group of one state with $J = 0$ (one state) and (4) the group with $J = 1$ (three states). Here and everywhere below the notation J stands for the total spin (or total momentum, for the $S(L = 0)$ -states) of the three-body ion. The states with $J = 2$ have the maximal energy, while the energy of the states from the fourth group is minimal. The corresponding splittings Δ_{12} , Δ_{23} and Δ_{34} can be found in Table VI for each bound state in the $pd\mu$ and $dt\mu$ ions.

The hyperfine structure of the ground state in the $pt\mu$ ion is completely different (see Table VII), since the spin of the triton equals $\frac{1}{2}$, while the spin of the deuteron (or deuterium nucleus) equals 1. In the case of the ground state in the $pt\mu$ ion one finds only eight spin states which are separated into three different groups: (1) the group of four states with $J = \frac{3}{2}$, (2) the group of two states with $J = \frac{1}{2}$ and (3) the group of two states with $J = \frac{1}{2}$. The group (1) has the maximal energy, while the energy of the states from the third group is minimal. The corresponding values of the hyperfine structure splittings in the ground state of the $pt\mu$ ion are $\Delta_{12} = 1.3400149 \cdot 10^7 \text{ MHz}$ and $\Delta_{23} = 3.3518984 \cdot 10^7 \text{ MHz}$.

In this Section we have investigated the hyperfine structure and determine the hyperfine structure splitting in the bound $S(L = 0)$ -states of the $pd\mu$, $pt\mu$ and $dt\mu$ ions. The first excited $S(L = 0)$ -state in the $dt\mu$ ion is traditionally designated by an additional asterisk, i.e. $(dt\mu)^*$. In such calculations we used the highly accurate expectation values of all inter-particle delta-functions obtained in recent computations [1]. In general, it is very interesting to compare the numerical values of the hyperfine structure splittings Δ_{12} , Δ_{23} and Δ_{34} for

different muonic ions (see Table VI).

VI. HYPERFINE STRUCTURE OF THE BOUND $S(L = 0)$ -STATES IN THE SYMMETRIC MUONIC MOLECULAR IONS

In this Section we consider the hyperfine structure splitting in the symmetric muonic molecular ions $pp\mu$, $dd\mu$ and $tt\mu$. As is well known there are five bound $S(L = 0)$ -states in these (symmetric) muonic molecular ions. The ground states are stable in each of these ions, while the excited $S(L = 0)$ -states are stable only in the heavy $dd\mu$ and $tt\mu$ ions. In general, the analysis of the hyperfine structure in symmetric systems is slightly more complicated than analogous analysis for non-symmetric systems/ions. On the other hand, the arising hyperfine structure is relatively simple and can be explained by using a few transparent physical ideas.

The general formula for the hyperfine structure splitting (or hyperfine splitting, for short) for an arbitrary three-body muonic molecular ion $aa\mu$ is written in the following form (in atomic units) (see, e.g., [14])

$$(\Delta H)_{h.s.} = \frac{2\pi}{3}\alpha^2 \frac{g_a g_a}{m_p^2} \langle \delta(\mathbf{r}_{aa}) \rangle (\mathbf{s}_a \cdot \mathbf{s}_a) + \frac{2\pi}{3}\alpha^2 \frac{g_a g_\mu}{m_p m_\mu} \langle \delta(\mathbf{r}_{a\mu}) \rangle (\mathbf{s}_a \cdot \mathbf{s}_\mu) + \frac{2\pi}{3}\alpha^2 \frac{g_a g_\mu}{m_p m_\mu} \langle \delta(\mathbf{r}_{a\mu}) \rangle (\mathbf{s}_a \cdot \mathbf{s}_\mu) \quad (14)$$

where $\alpha = \frac{e^2}{\hbar c}$ is the fine structure constant, m_μ and m_p are the muon and proton masses, respectively. The factors g_μ and g_a are the corresponding g -factors. The expression for $(\Delta H)_{h.s.}$ is, in fact, an operator in the total spin space which has the dimension $(2s_a + 1)^2(2s_\mu + 1)$. Since the second and third terms in Eq.(1) are identical, then we can reduce Eq.(14) to the form

$$(\Delta H)_{h.s.} = \frac{2\pi}{3}\alpha^2 \frac{g_a g_a}{m_p^2} \langle \delta(\mathbf{r}_{aa}) \rangle (\mathbf{s}_a \cdot \mathbf{s}_a) + \frac{2\pi}{3}\alpha^2 \frac{g_a g_\mu}{m_p m_\mu} \langle \delta(\mathbf{r}_{a\mu}) \rangle (\mathbf{S}_{aa} \cdot \mathbf{s}_\mu) \quad (15)$$

where $\mathbf{S}_{aa} = (\mathbf{s}_a + \mathbf{s}_a)$ is the total spin of the pair of identical particles (the two nuclei of the hydrogen isotopes), i.e. p , d and t .

The formula, Eq.(15), allows one to make a few qualitative predictions about the hyperfine structure of the symmetric muonic molecular ions. First, it is clear that the classifications of the levels of hyperfine structure must be based on the total spin of the two ‘symmetric’

nuclei \mathbf{S}_{aa} . The absolute values of the spin \mathbf{S}_{aa} are always non-negative integer numbers, i.e. $|\mathbf{S}_{aa}| = 0, 1, 2, \dots$. For instance, in the case of two protons p and/or two tritons t one finds $|\mathbf{S}_{aa}| = 0, 1$, while for the two deuterons $|\mathbf{S}_{aa}| = 0, 1, 2$. The hyperfine energy of this state with $J = 0$ is determined only by the first term in Eq.(15) which is very small, since the expectation values $\langle \delta(\mathbf{r}_{aa}) \rangle$ in all muonic molecular ions are very small. As follows from actual computations all these values are less than $4 \cdot 10^{-5}$ (in muon atomic units). Briefly, we can say that the energy of this hyperfine state (with $J = \frac{1}{2}$) is determined by the spin-spin interaction between the two heavy nuclei (muon's spin does not contribute). The overall contribution from the first term in Eq.(15) rapidly (exponentially) decreases when the mass of the heavy particle increases. Formally, the first term in Eq.(15) is very small already for the $pp\mu$ ion. However, for the $dd\mu$ and $tt\mu$ ions its contribution is negligible. This means that in the first approximation the hyperfine structure of the symmetric muonic molecular ions can be explained by using only one term for the muon-nuclear spin interaction. This leads to some 'additional' symmetry observed for the actual levels of hyperfine structure of heavy ions (see below).

As is well known the spin of the negatively charged muon μ^- equals $\frac{1}{2}$ and the spins of the proton p and triton t also equal $\frac{1}{2}$. Therefore, the hyperfine structure of the $pp\mu$ and $tt\mu$ ions must include eight levels which form three following groups: (1) the group of four spin states with $J = \frac{3}{2}$, (2) the upper group of two states with $J = \frac{1}{2}$ and (3) the lower group of two states with $J = \frac{1}{2}$. The classification is true for the excited $S(L=0)$ -state in the $tt\mu$ ion. Here and everywhere below the notation J stands for the total spin (or total momentum) of the three-body system/ion, since $\mathbf{J} = \mathbf{L} + \mathbf{S} = \mathbf{S}$ for the $S(L=0)$ -states).

The hyperfine structure of the $dd\mu$ ion is substantially different. In the $dd\mu$ ion one finds eighteen levels of hyperfine structure which are separated into five different groups: one group with $J = \frac{5}{2}$ (six states), two different groups of states (upper and lower groups) with $J = \frac{3}{2}$ (four states in each), two different groups of states (upper and lower groups) with $J = \frac{1}{2}$ (two states in each).

In our calculations of the hyperfine structure we have used the following numerical values for the constants and factors in Eq.(15): $\alpha = 7.297352586 \cdot 10^{-3}$, $g_\mu = -2.0023218396$ [16] and $m_p = 1836.152701m_e$, $m_\mu = 206.768262m_e$. The g -factors for the proton, deuteron and triton are determined from the formulas: $g_p = \frac{\mathcal{M}_d}{I_p}$, $g_d = \frac{\mathcal{M}_d}{I_d}$ and $g_t = \frac{\mathcal{M}_t}{I_t}$, where $\mathcal{M}_p = 2.792847386$, $\mathcal{M}_d = 0.857438230$ and $\mathcal{M}_t = 2.97896247745$ are the magnetic moments

(in nuclear magnetons) of the proton, deuteron and triton, respectively. Here the spins of the proton, deuteron and triton are designated in by the letter I with the corresponding index: $I_p = \frac{1}{2}$, $I_d = 1$ and $I_t = \frac{1}{2}$. In Eqs.(14) - (15) these values are designated differently. In highly accurate computations of the expectation values of delta-functions we have used the following masses of the deuteron and triton: $m_d = 3680.483014 m_e$ and $m_t = 5496.92158 m_e$. These masses are often used in modern highly accurate calculations of muonic molecular ions (see, e.g., [1]).

The convergence of the expectation values of the nuclear-nuclear (or $pp-$) and nuclear-muonic (or $p\mu-$) delta-functions is illustrated in Table VIII for the $pp\mu$ ion. The convergence of these expectation values for other bound $S(L=0)$ -states in the $dd\mu$ and $tt\mu$ ions is very similar to the results presented in Table VIII for the $pp\mu$ ion. The hyperfine structure and energy splittings between the corresponding levels for all five bound $S(L=0)$ -states in the three muonic molecular ions $pp\mu$, $dd\mu$ and $tt\mu$ can be found in Tables IX and X. In atomic physics these values are traditionally given in MHz . The corresponding conversion factor is $6.57968392061 \cdot 10^9 MHz/a.u.$ In Tables IX and X the excited states are designated by the asterisk used as the upper index, e.g., $(dd\mu)^*$ and $(tt\mu)^*$. Such a system of notation is often used for muonic molecular ions.

Tables IX and X contain both the energies of the levels of hyperfine structure (ϵ_J) and hyperfine structure splitting ($\Delta(J_1 \rightarrow J_2)$). As we have predicted (see above) one of the hyperfine levels has a very small energy. As follows from Tables IX and X this level corresponds to $J = \frac{1}{2}$. In the $tt\mu$ ion the hyperfine energies of this state are $\approx 11.0591 MHz$ and $\approx 12.4307 MHz$ for the ground and first excited states, respectively. In the $dd\mu$ ion the energies of the analogous levels are $6.8996 MHz$ and $4.7378 MHz$, respectively. Briefly, this means that the overall contribution of the nuclear-nuclear spin interaction is very small for the both $dd\mu$ and $tt\mu$ ions. This directly follows from the known fact (see, e.g., [17]) that the expectation values of nuclear-nuclear delta-functions are very small. For instance, for the $dd\mu$ and $tt\mu$ ions the expectation values of nuclear-nuclear delta-functions are $\langle \delta_{dd} \rangle \approx 2.43871205 \cdot 10^{-6} (m.a.u.)$, $\langle \delta_{dd} \rangle \approx 1.67460229 \cdot 10^{-6} (m.a.u.)$, $\langle \delta_{tt} \rangle \approx 2.15893994 \cdot 10^{-7} (m.a.u.)$ and $\langle \delta_{tt} \rangle \approx 2.42670033 \cdot 10^{-7} (m.a.u.)$, for the ground and excited states, respectively. Finally, the observed hyperfine structure of these two ions is mainly (99.9999 %) related to the muon-nuclear spin interactions only. In the $pp\mu$ ion the situation is slightly different, but even for this ion the overall contribution of the muon-nuclear spin interaction(s)

is substantially larger than the contribution from the nuclear-nuclear spin interaction.

VII. CONCLUSION

Thus, we have determined the total energies of the twenty one bound states in the six muonic molecular ions $pp\mu, pd\mu, pt\mu, dd\mu, dt\mu$ and $tt\mu$. The angular momentum of these bound states equals $L = 0$, $L = 1$ and $L = 2$. Our calculations of the bound state energies in this study have been performed with the improved particle masses known from recent high-energy experiments. The highly accurate wave functions of muonic molecular ions are needed to determine the expectation values of some operators. These expectation values are of interest in numerous applications related to the muonic molecular ions. Currently, all muonic molecular ions can be created in real experiments and their various properties can be measured to very good accuracy. Therefore, we can compare the predicted (or computed) values of the bound state properties with their actual (or observed) values. In general, the analysis of these three-body systems is significantly more interesting and informative than the traditional analysis of the two-electron atoms and ions.

The hyperfine structure of all nine bound $S(L = 0)$ -states of the $pp\mu, pd\mu, pt\mu, dd\mu, dt\mu$ and $tt\mu$ has also been investigated. In our calculations of hyperfine structure and hyperfine structure splittings for each of these states we used the highly accurate expectation values of the interparticle delta-functions. The hyperfine structure splittings of the ground states of each of these ions (see Tables VI, VII, IX and X) can directly be measured in modern experiments.

Appendix

In this Appendix we briefly discuss the history of the bound state computations of muonic molecular ions. Note that the interest to these ions was always closely related to the problems of muon-catalyzed fusion of the nuclear reactions. The first numerical computations of the bound states in three-body muonic molecular ions were performed by Belyaev et al in 1959 [18]. By using a very simple adiabatic (but non-variational!) procedure they were able to find 20 bound states in six ions $pp\mu, pd\mu, pt\mu, dd\mu, dt\mu$ and $tt\mu$. Unfortunately, due to lack of good computers at that time the overall accuracy of the procedure used in [18] was very low and the authors could not confirm the boundness of the excited $P^*(L = 1)$ -states (or (1,1)-states) in

the $dd\mu$ and $dt\mu$ ions. It was concluded only that, if such states are bound, then they are very weakly bound. The binding energy of these two states was expected to be smaller than 4.5 eV, i.e. smaller than the binding energy of a typical hydrogen molecule. Immediately after publication of [18] an intense stream of speculations started about a possible interference (or resonance) between the formation of excited $P^*(L = 1)$ -states (or (1,1)-states) in the $dd\mu$ and $dt\mu$ muonic molecular ions and different transitions in surrounding molecules (see, e.g., [19] and references there in).

In the middle of 1960's Halpern [20], Carter [21], [22] and Delves and Kalotas [23] published their papers with the results of variational computations obtained for some bound states in the muonic molecular ions. In particular, Halpern [20] considered the bound $P(L = 1)$ -states in the symmetric $pp\mu$, $dd\mu$, $tt\mu$ ions. The paper of Delves and Kalotas has a great methodological interest, since 99 % of all modern methods for highly accurate computations of Coulomb three-body systems are based on that work. At the same time a number of experiments have been performed by Bystritskii et al (see [24] and [25] and references therein). They worked with μ^- -muons which were slowing down in liquid deuterium and deuterium-tritium mixture. Finally, it was found that one muon can catalyze approximately 10 - 20 (d, d)-nuclear reactions in liquid deuterium (D_2) and 90 - 110 (d, t)-reactions in the liquid equimolar deuterium-tritium mixture ($D_2 : T_2 = 1:1$). Such very large numbers of nuclear reactions catalyzed by one muon can be explained only by the resonance (or very fast) formation of $dd\mu$ and $dt\mu$ muonic molecular ions. Correspondingly, the related processes were called 'resonance' muon-catalyzed fusion of nuclear reactions, in contrast with the 'regular' muon-catalyzed fusion observed in [26].

Those experimental works produced a great interest to study the weakly-bound states in the $dd\mu$ and $dt\mu$ ions. The main goal of all following computations was to determine the binding energies of the weakly-bound $P^*(L = 1)$ -states in the $dd\mu$ and $dt\mu$ ions to the accuracy $\approx 1 \cdot 10^{-3}$ eV (or approximately 10 K). At that time a large number of bound state computations for muonic molecular ions were performed with the use of the adiabatic (but non-variational!) method [27]. The first variational computations of all bound $S(L = 0)$ - and $P(L = 1)$ -states in muonic molecular ions have been conducted in [28] and [29]. Later, we have substantially improved the accuracy of such computations [30] and were able to calculate the bound $D(L = 2)$ -states in these ions [31]. Since then we have performed a number of different computations of the bound $D(L = 2)$ -states in the $dd\mu$, $dt\mu$ and

$tt\mu$ ion. The total energy of the $dt\mu$ ion [32] is the only result obtained for these states outside of our group. However, in the middle of 1980's the masses of all particles involved in the muonic molecular ions were determined to much better accuracy. In addition to this, it became finally clear that the main restriction of the resonance muon-catalyzed fusion is directly related to the muon sticking coefficient to the ^4He nucleus, or with its inverse value which equals to the number of nuclear reactions catalyzed by one muon in the equimolar deuterium-tritium mixture. It appears that such a number (150 - 160) was very close to the value obtained earlier [24] and [25]. It was also shown that even 200 nuclear fusions per one muon in the equimolar deuterium-tritium (liquid) mixture is in 12 - 15 times less than it is needed for theoretical break-even and ≈ 55 - 65 times smaller than necessary for actual break-even (see discussion and references in [33]).

After these publications the overall interest to the resonance muon-catalyzed fusion rapidly went down. Nevertheless, in the middle of 1990's we have performed a series of highly accurate computations of the muonic molecular ions [34], [35]. These works were originally stimulated by the development of the theory of bound states in the Coulomb three-body systems with unit charges. Later, I have wrote the code to determine the energy and some other properties of the $F(L=3)$ -state in the $tt\mu$ ion. In our calculations performed around 2001 - 2003 we have used the advanced Fortran pre-translator written by D.H. Bailey [36], [37]. Around that time another paper was published on highly accurate bound state computations of the three-body muonic molecular ions [38]. In [1] we have used very large basis sets and performed an accurate optimization of the non-linear parameters of our method. The paper [1] contains the most accurate values of the total (and binding energies) of all 22 bound states in the six muonic molecular ions $pp\mu$, $pd\mu$, $pt\mu$, $dd\mu$, $dt\mu$ and $tt\mu$. In this study we wanted to recalculate some of these systems by using the new values of the particle masses.

Note in conclusion that despite an obvious failure of the resonance muon-catalyzed fusion in the D:T mixture the muon-catalysis of the nuclear reactions is not a closed problem. In this area one still finds dozens of unsolved, approximately and wrongly solved problems. One of such problems is the current (very large) deviation between theoretical and experimental fusion rates in the $pt\mu$ ion. Other open problems include accurate evaluations of the fusion rates and muon sticking probabilities for some rotationally excited states, probabilities of

excitations (and de-excitations) of muon-molecular ions, etc.

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TABLE I: The total energies (E) of the bound $S(L = 0)$ -states in the symmetric muonic molecular ions in muon-atomic units ($m_\mu = 1, \hbar = 1, e = 1$). N designates the number of basis functions used in Eq.(2).

N	$E(pp\mu)$	$E(dd\mu)$	$E(tt\mu)$
3300	-0.494386 815212 835026 521839	-0.531111 132193 187917 45	-0.546374 225613 816728 844
3500	-0.494386 815212 835026 522038	-0.531111 135402 386449 61	-0.546374 225613 816728 849
3700	-0.494386 815212 835026 522184	-0.531111 135402 386450 59	-0.546374 225613 816728 855
3840	-0.494386 815212 835026 522266	-0.531111 135402 386451 22	-0.546374 225613 816728 856
∞	-0.494386 815212 835026 52250(10)	-0.531111 135402 386455(2)	-0.546374 225613 816728 90(3)
N	$E(pd\mu)$	$E(pt\mu)$	$E(dt\mu)$
3300	-0.512 711 792 481 703 484	-0.519 880 085 704 058 459	-0.538 594 971 709 480 710
3500	-0.512 711 792 481 703 573	-0.519 880 085 704 058 570	-0.538 594 971 709 480 718
3700	-0.512 711 792 481 703 647	-0.519 880 085 704 058 670	-0.538 594 971 709 480 724
3840	-0.512 711 792 481 703 670	-0.519 880 085 704 058 711	-0.538 594 971 709 480 730
∞	-0.512 711 792 481 703 85(4)	-0.519 880 085 704 058 87(4)	-0.538 594 971 709 480 79(2)
N	$E^*(dd\mu)$	$E^*(dt\mu)$	$E^*(tt\mu)$
3300	-0.47970 63771 01901 40596	-0.488 065 354 215 765 737	-0.49676 28898 97946 30625
3500	-0.47970 63771 01901 40638	-0.488 065 354 215 765 800	-0.49676 28898 97946 30709
3700	-0.47970 63771 01901 40667	-0.488 065 354 215 765 843	-0.49676 28898 97946 30786
3840	-0.47970 63771 01901 40689	-0.488 065 354 215 765 860	-0.49676 28898 97946 30823
∞	-0.47970 63771 01901 4080(3)	-0.488 065 354 215 765 98(4)	-0.49676 28898 97946 314(3)

TABLE II: The total energies (E) of the bound $P(L = 1)$ -states in the symmetric muonic molecular ions in muon-atomic units ($m_\mu = 1, \hbar = 1, e = 1$). N designates the number of basis functions used in Eq.(2).

N	$E(pp\mu)$	$E(dd\mu)$	$E(tt\mu)$
3300	-0.468 458 430 358 808 027 03	-0.513 623 952 704 526 3269	-0.533 263 445 209 533 2938
3500	-0.468 458 430 358 808 031 55	-0.513 623 952 704 526 3342	-0.533 263 445 209 533 3070
3700	-0.468 458 430 358 808 035 14	-0.513 623 952 704 526 3387	-0.533 263 445 209 533 3189
3840	-0.468 458 430 358 808 037 51	-0.513 623 952 704 526 3407	-0.533 263 445 209 533 3254
∞	-0.468 458 430 358 808 045(3)	-0.513 623 952 704 526 39(3)	-0.533 263 445 209 533 38(3)
N	$E(pd\mu)$	$E(pt\mu)$	$E(dt\mu)$
3300	-0.490 664 164 603 504 64	-0.499 492 024 990 190 10	-0.523 191 452 003 587 60
3500	-0.490 664 164 603 507 57	-0.499 492 024 990 191 53	-0.523 191 452 003 588 67
3700	-0.490 664 164 603 510 41	-0.499 492 024 990 192 53	-0.523 191 452 003 589 54
3840	-0.490 664 164 603 511 76	-0.499 492 024 990 192 96	-0.523 191 452 003 590 17
∞	-0.490 664 164 603 515(1)	-0.499 492 024 990 195(1)	-0.523 191 452 003 593(1)
N	$E^*(dd\mu)$	$E^*(dt\mu)$	$E^*(tt\mu)$
3300	-0.473 686 731 121 137 629	-0.481 991 527 054 2451	-0.489 908 663 057 013 5630
3500	-0.473 686 731 121 137 765	-0.481 991 527 054 3644	-0.489 908 663 057 013 6844
3700	-0.473 686 731 121 137 946	-0.481 991 527 054 4505	-0.489 908 663 057 013 8018
3840	-0.473 686 731 121 138 063	-0.481 991 527 054 4894	-0.489 908 663 057 013 8571
∞	-0.473 686 731 121 138 5(3)	-0.481 991 527 054 9(3)	-0.489 908 663 057 014 5(2)

TABLE III: The total energies (E) of the bound $D(L = 2)$ -states of the the $dd\mu$, $tt\mu$ and $dt\mu$ muonic molecular ions in muon atomic units. N designates the number of basis functions used in Eq.(2).

N	$E(dd\mu)$	$E(tt\mu)$	N	$E(dt\mu)$
2800	-0.488 708 327 4382	-0.512 568 647 4651	3900	-0.500 118 078 7334
3000	-0.488 708 327 5083	-0.512 568 647 6583	4200	-0.500 118 078 7337
3200	-0.488 708 327 5460	-0.512 568 647 8022	4500	-0.500 118 078 7338
3400	-0.488 708 327 5584	-0.512 568 647 9152	4800	-0.500 118 078 7338
3600	-0.488 708 327 5715	-0.512 568 648 0085	5100	-0.500 118 078 7338
∞	-0.488 708 327 598(3)	-0.512 568 648 210(5)	∞	-0.500 118 078 7338(1)

TABLE IV: The bound state properties X computed for the ground $S(L = 0)$ -state and excited $S^*(L = 0)$ -state in the $pd\mu$ and $dt\mu$ muonic molecular ions (in muon-atomic units).

X	$pd\mu(S(L = 0)\text{--state})$	$dt\mu(S(L = 0)\text{--state})$	$dt\mu(S^*(L = 0)\text{--state})$
$\langle r_{31}^{-1} \rangle$	0.6411463600638491(1)	0.7227000026976390(3)	0.5146887255965181(3)
$\langle r_{32}^{-1} \rangle$	0.7533736114443716(1)	0.7583156054974041(3)	0.7053753065541911(3)
$\langle r_{21}^{-1} \rangle$	0.3690963865448171(3)	0.4038256647760819(5)	0.2439333237191783(6)
$\langle r_{31} \rangle$	2.451487643610344(2)	2.117912271227347(3)	3.933236044506724(3)
$\langle r_{32} \rangle$	2.087699160470998(2)	2.023720516217468(3)	2.738751054881910(3)
$\langle r_{21} \rangle$	3.100710462458351(3)	2.747914171742117(5)	5.161229304527515(5)
$\langle r_{31}^2 \rangle$	8.033494559453071(3)	5.881854047519130(4)	22.39719714570313(5)
$\langle r_{21}^2 \rangle$	10.829021567566262(4)	8.2873255690653121(6)	30.631304593819174(6)
$\langle r_{32}^3 \rangle$	20.6547098820345(2)	17.4696971262928(3)	65.2551287149941(3)
$\langle r_{21}^3 \rangle$	42.147966883621(4)	27.208344987497(5)	201.45182645373(6)
$\langle -\frac{1}{2}\nabla_1^2 \rangle$	0.2806191821887450(7)	0.3910764626134503(9)	0.3836327048408983(9)
$\langle -\frac{1}{2}\nabla_2^2 \rangle$	0.3674608971218589(7)	0.4218837688718115(9)	0.4476331876944995(9)
$\langle -\frac{1}{2}\nabla_3^2 \rangle$	0.46041133009768349(4)	0.50069529322880649(5)	0.50035758500774130(6)

TABLE V: The convergence of the $\langle\delta_{32}\rangle$, $\langle\delta_{31}\rangle$ and $\langle\delta_{21}\rangle$ expectation values for the ground (bound) $S(L=0)$ -state of the $pd\mu$ molecular ion (in muon-atomic units).

N	$\langle\delta_{32}\rangle$	$\langle\delta_{31}\rangle$	$\langle\delta_{21}\rangle$
3300	$1.73456203087 \cdot 10^{-1}$	$1.17709732798 \cdot 10^{-1}$	$1.46169407 \cdot 10^{-5}$
3500	$1.73456202965 \cdot 10^{-1}$	$1.17709733128 \cdot 10^{-1}$	$1.46169370 \cdot 10^{-5}$
3700	$1.73456202754 \cdot 10^{-1}$	$1.17709733014 \cdot 10^{-1}$	$1.46169377 \cdot 10^{-5}$
3840	$1.73456202768 \cdot 10^{-1}$	$1.17709733160 \cdot 10^{-1}$	$1.46169383 \cdot 10^{-5}$

TABLE VI: The levels of hyperfine structure ϵ and hyperfine structure splittings Δ in the bound $S(L=0)$ -states of the $pd\mu$ and $dt\mu$ ions (in MHz).

$\epsilon_{J=2}(pd\mu)$	$1.2519350851 \cdot 10^7$	—	—
$\epsilon_{J=1}(pd\mu)$	$9.3058194294 \cdot 10^6$	$\Delta(J=2 \rightarrow J=1)$	$3.2135314217 \cdot 10^6$
$\epsilon_{J=0}(pd\mu)$	$-2.1222395094 \cdot 10^7$	$\Delta(J=1 \rightarrow J=0)$	$3.0528214524 \cdot 10^7$
$\epsilon_{J=1}(pd\mu)$	$-2.3097272483 \cdot 10^7$	$\Delta(J=0 \rightarrow J=1)$	$1.8748773889 \cdot 10^6$
$\epsilon_{J=2}(dt\mu)$	$1.8919590437 \cdot 10^7$	—	—
$\epsilon_{J=1}(dt\mu)$	$1.5985479092 \cdot 10^6$	$\Delta(J=2 \rightarrow J=1)$	$2.9341113453 \cdot 10^6$
$\epsilon_{J=0}(dt\mu)$	$-3.4439378258 \cdot 10^7$	$\Delta(J=1 \rightarrow J=0)$	$5.0424857350 \cdot 10^7$
$\epsilon_{J=1}(dt\mu)$	$-3.6038337067 \cdot 10^7$	$\Delta(J=0 \rightarrow J=1)$	$1.5989588085 \cdot 10^6$
$\epsilon_{J=2}(dt\mu)^*$	$1.8609555434 \cdot 10^7$	—	—
$\epsilon_{J=1}(dt\mu)^*$	$1.6554331952 \cdot 10^6$	$\Delta(J=2 \rightarrow J=1)$	$2.0552234821 \cdot 10^6$
$\epsilon_{J=0}(dt\mu)^*$	$-3.4859818025 \cdot 10^7$	$\Delta(J=1 \rightarrow J=0)$	$5.1414149977 \cdot 10^7$
$\epsilon_{J=1}(dt\mu)^*$	$-3.5950318334 \cdot 10^7$	$\Delta(J=0 \rightarrow J=1)$	$1.0905003094 \cdot 10^6$

TABLE VII: The levels of hyperfine structure ϵ and hyperfine structure splittings Δ in the ground $S(L = 0)$ –state of the $pt\mu$ ion (in MHz).

$\epsilon_{J=\frac{3}{2}}(pt\mu)$	$1.5079820356 \cdot 10^7$	—	—
$\epsilon_{J=\frac{1}{2}}(pt\mu)$	$1.6796717260 \cdot 10^6$	$\Delta(J = \frac{3}{2} \rightarrow J = \frac{1}{2})$	$1.3400148630 \cdot 10^7$
$\epsilon_{J=\frac{1}{2}}(pt\mu)$	$-3.1839312439 \cdot 10^7$	$\Delta(J = \frac{1}{2} \rightarrow J = \frac{1}{2})$	$3.3518984165 \cdot 10^7$

TABLE VIII: The convergence of the $\langle\delta_{p\mu}\rangle$ and $\langle\delta_{pp}\rangle$ expectation values for the ground (bound) $S(L = 0)$ –state of the $pp\mu$ molecular ion (in muon-atomic units).

N	$\langle\delta_{31}\rangle$	$\langle\delta_{21}\rangle$
3300	$1.315008614364 \cdot 10^{-1}$	$3.9370034861 \cdot 10^{-5}$
3500	$1.315008614369 \cdot 10^{-1}$	$3.9370034722 \cdot 10^{-5}$
3700	$1.315008614374 \cdot 10^{-1}$	$3.9370034782 \cdot 10^{-5}$
3840	$1.315008614378 \cdot 10^{-1}$	$3.9370034773 \cdot 10^{-5}$

TABLE IX: The hyperfine structure and hyperfine structure splitting of the bound $S(L = 0)$ –states of the $pp\mu$ and $tt\mu$ ions (in MHz).

	$pp\mu$	$tt\mu$	$(tt\mu)^*$
$\epsilon_{J=\frac{3}{2}}$	$1.256448515 \cdot 10^7$	$1.736310113 \cdot 10^7$	$1.510018118 \cdot 10^7$
$\epsilon_{J=\frac{1}{2}}$	$1.772596177 \cdot 10^3$	$1.105911127 \cdot 10^1$	$1.243070661 \cdot 10^1$
$\epsilon_{J=\frac{1}{2}}$	$-2.513074289 \cdot 10^7$	$-3.472621366 \cdot 10^7$	$-3.020037480 \cdot 10^7$
$\Delta(\frac{3}{2} \rightarrow \frac{1}{2})$	$1.256271251 \cdot 10^7$	$1.735309024 \cdot 10^7$	$1.510016875 \cdot 10^7$
$\Delta(\frac{1}{2} \rightarrow \frac{1}{2})$	$2.513251549 \cdot 10^7$	$3.472622472 \cdot 10^7$	$3.020038723 \cdot 10^7$

TABLE X: The hyperfine structure and hyperfine structure splitting of the bound $S(L = 0)$ -states of the $dd\mu$ ion (in MHz).

	$dd\mu$	$(dd\mu)^*$
$\epsilon_{J=\frac{5}{2}}$	$4.656669271 \cdot 10^6$	$4.023227167 \cdot 10^6$
$\epsilon_{J=\frac{3}{2}}$	$2.328339810 \cdot 10^6$	$2.011617137 \cdot 10^6$
$\epsilon_{J=\frac{1}{2}}$	$6.899579465 \cdot 10^0$	$4.737788941 \cdot 10^0$
$\epsilon_{J=\frac{1}{2}}$	$-4.656669271 \cdot 10^6$	$-4.023227167 \cdot 10^6$
$\epsilon_{J=\frac{3}{2}}$	$-6.985012530 \cdot 10^6$	$-6.034846672 \cdot 10^6$
$\Delta(\frac{5}{2} \rightarrow \frac{3}{2})$	$2.328329461 \cdot 10^6$	$2.01161003 \cdot 10^6$
$\Delta(\frac{3}{2} \rightarrow \frac{1}{2})$	$2.328332911 \cdot 10^6$	$2.01161239 \cdot 10^6$
$\Delta(\frac{1}{2} \rightarrow \frac{1}{2})$	$4.656676170 \cdot 10^6$	$4.02323191 \cdot 10^6$
$\Delta(\frac{1}{2} \rightarrow \frac{3}{2})$	$2.328343259 \cdot 10^6$	$2.01161951 \cdot 10^6$